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PREDICTION OF WOOD PELLETS COMBUSTION BY THE EXTENDED DISCRETE ELEMENT METHOD (XDEM)

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Abstract. The objective of this contribution is to predict the combustion of wood pellets in an domestic oven by the Extended Discrete Element Method (XDEM). It poses insofar a challenge as various physical processes such as combustion in conjunction with dynamic motion of pellets all emerged in a gas phase. In order to allow describing the complex interaction between the above-mentioned processes, a coupled Euler-Lagrange approach was chosen. The pellets are treated as discrete cylindrical elements of which the dynamics are tracked with the classical Discrete-Element-Method. It is extended by the thermodynamic state for each pellet to predict both temperature and species distribution inside a pellet during combustion, and thus, allows tracking the reaction progress. Thermal conversion of pellets includes heating, drying, pyrolysis and char combustion. Feeding of particles is taken into account by batches as applied under industry-like operation. The flow of combustion air with its temperature and species distribution is predicted by classical CFD approaches. The pellets interact with the surrounding gas phase via heat, mass and momentum transfer which is taken into account by relevant empirical correlations.

Pellets form a packed bed at the bottom of an cylindrical enclosure through which combustion air is provided. While streaming through the void space between the pellets, intensive heat and mass transfer takes place. Combustion air provide necessary oxygen for combustion while hot pellets transfer heat to the air and thus heating it up. Pellets shrink according to the reaction progress and thus initiate motion of the packed bed. It is also amplified by the batch-wise feeding of pellets matching the given mass flow e.g. combustion rate that introduces significant temporal variations of the entire process. The following figure depicts both surface temperature of pellets and gas velocity.

1 INTRODUCTION

Contrary to continuum models an alternative approach considers the solid phase as discrete, while the flow of liquids or gases is treated as a continuum phase in the void space between the particles, and therefore, is labelled the Combined Continuum and Discrete Model (CCDM) [1, 2, 3, 4]. Due to a discrete description of the solid phase, constitutive relations are omitted, and therefore, leads to a better understanding of the fundamentals. This was also concluded by Zhu et al. [5] and Zhu et al. [6] during a review on particulate flows modelled with the CCDM approach. Based on this approach Sheng et al. [7] investigated into the micro-scale heat transfer of packed beds and micro-fibrous entrapped catalysts and concluded that the thermal resistance of the contact points account for more than 90 % of the total resistance. Similarly, Kon et al. [8] modelled the liquid flow in the lower part of a blast furnace by the MPS method. CCDM has seen a mayor development in last two decades and describes motion of the solid phase by the Discrete Element Method (DEM) on an individual particle scale and the remaining phases are treated by the Navier-Stokes equations.

However, current CCDM approaches should be extended to a truly multi-phase flow behaviour as opposed to the Volume-of-Fluid method and the multi-phase mixture model [9]. Furthermore, particle shapes other than spherical geometries have to be taken into account to meet engineering needs according to Zhu et al. [5] and Zhu et al. [6]. This efforts should ideally be complemented by poly-disperse particle systems as employed by Peters and Dziugys [10]. All these efforts should contribute to a general link between continuum and discrete approaches so that results are quantified for process modelling.

2 NUMERICAL TECHNIQUE

A novel technique referred to as Extended Discrete Element Method (XDEM) [11] has emerged only recently that offers a significant advancement for multi-physics applications. It is based on a coupled discrete and continuous i.e. Lagrange-Euler simulation concept. XDEM treats the solid phase representing the particles and the fluid phase or a structure as two distinguished entities that are coupled through heat, mass and momentum transfer. An outstanding feature of the numerical concept is that each particle in addition to its position and orientation in time and space is described by its thermodynamic state e.g. temperature and reaction progress. The thermodynamic state is described by one-dimensional and transient differential conservation equations for mass, energy and momentum for each individual particle and thus, characterizes the overall behaviour of the reactor as the sum of all particle processes. Predicted results for all individual particles allow a detailed analysis of the reaction process. Through predicting position and orientation of all particles their arrangement in space is known that determines the 3-dimensional distribution of void space between the particles. This essentially represents a porous structure through which the fluid e.g. liquid or gas streams. The fluid is in contact with the surface of the particles and determines heat and mass exchange between

the particles surface and the fluid i.e. temperature and composition in the vicinity of the particle. In order to predict flow through the interstitial space a classical CFD approach is preferred for which the software framework of OpenFoam is employed. Its library offers a large selection of solves for different applications and allows as an open-source software a tailored development of solvers suiting the needs of the above-mentioned applications. Hence, the proposed methodology provides a high degree of resolution ranging from scales within a particle to the continuum phase as global dimensions and offers superior features as compared to traditional and pure continuum mechanics approaches. The latter does not include detailed information on a particulate scale that has to be compensated for by empirical correlations such as distribution of void space in a packed or moving bed. For a more detailed description the reader is referred to Peters et al. [12, 13, 14].

3 RESULT AND DISCUSSION

Fig.1 illustrates the mass fraction of volatile matter during conversion of wood particles in the stove. At the beginning of simulation due to solely drying processes, only water vapour is produced and transferred to the gas phase. This procedure continues until the total amount of water is evaporated which takes around 40 s. Afterwards the thermal devolatilisation of wood commences and gas volatiles of CO_2, CO, CH_4, H_2O and H_2 are delivered and transferred to the gas phase. This process lasts until 120 s. In this moment the pyrolysis is terminated and the gasification as well as combustion processes are started. The gas compositions released by the wood are mixed with the oxygen and combusted above the bed in the chamber. These exothermic reactions generate required energy at the end of pyrolysis leading to char gasification. In addition, the oxygen can go through the pores of particles leading to char combustion at high temperature. However, due to mass transfer of the volatiles and lack of CO_2 and H_2O at the end of pyrolysis, the gasification occurs due to reaction with released CO_2 by char combustion. Since during pyrolysis the produced volatiles prevent the oxygen to enter the particle, the char combustion takes place after pyrolysis. Furthermore, it is shown in fig.2 the behaviour of solid materials during conversion process. At the beginning, wood appears as a sole solid material while drying is taking place. When the pyrolysis commences, the wood is depleted and it is converted partly to the solid char. This procedure continues until around 120 s where the wood is totally consumed and the produced char matter start to be gasified and combusted. Also fig.3 represents the behaviour of liquids during conversion of wood particles in the oven. While the water content of particles are vaporized during drying, and subsequently with onset of pyrolysis, tar is formed by wood devolatilisation. The produced tar is transferred to the gas phase and is combusted with oxygen above the bed leading to generation of carbon monoxide and hydrogen inside the oven. Additionally, fig.4 shows the temperature distribution of particles and gas phase at 250 s. It represents the centre slice inside the chamber showing the gas temperature and the cylinders are solid particles with their surface temperature. The high temperature of particles is due to char combustion leading to generate a vast amount of energy. In the gas phase, the high

temperature region above the bed represents the flame generated due to the combustion of volatiles. which is due to the reactions between the volatiles and injected oxygen through the secondary air inlet.

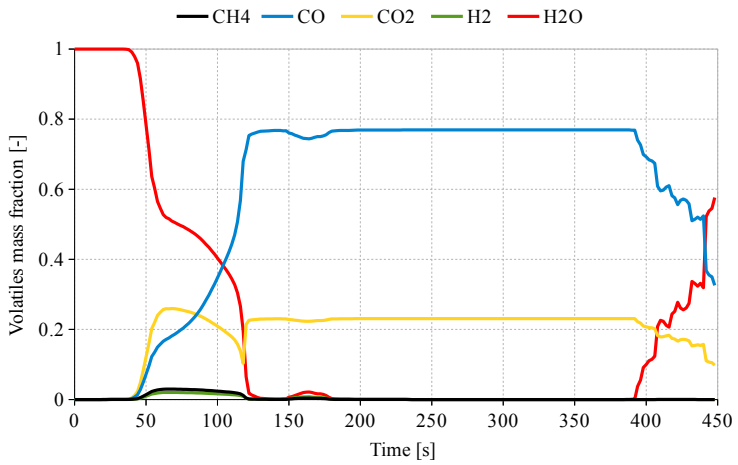

Figure 1: Mass fraction of released gas compositions of the bed

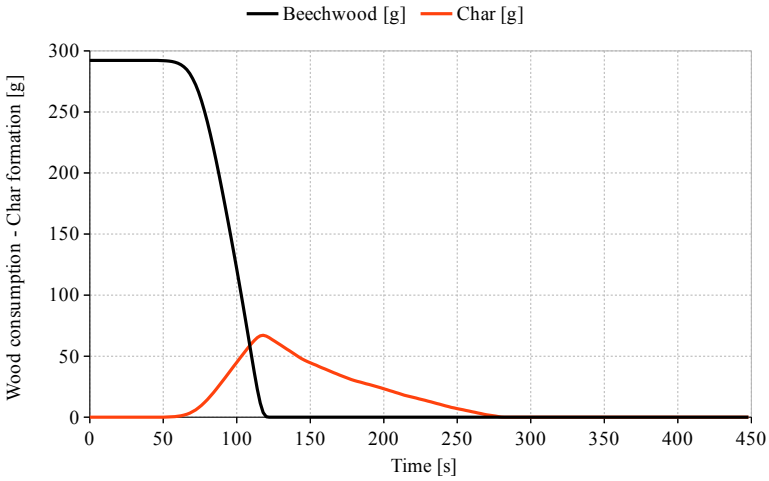

Figure 2: Wood consumption and char formation of the bed

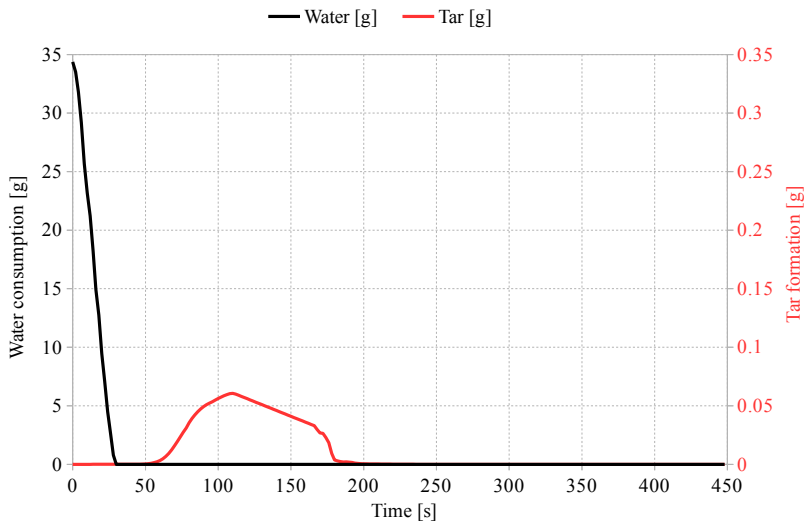

Figure 3: Water content consumption and tar formation of the bed

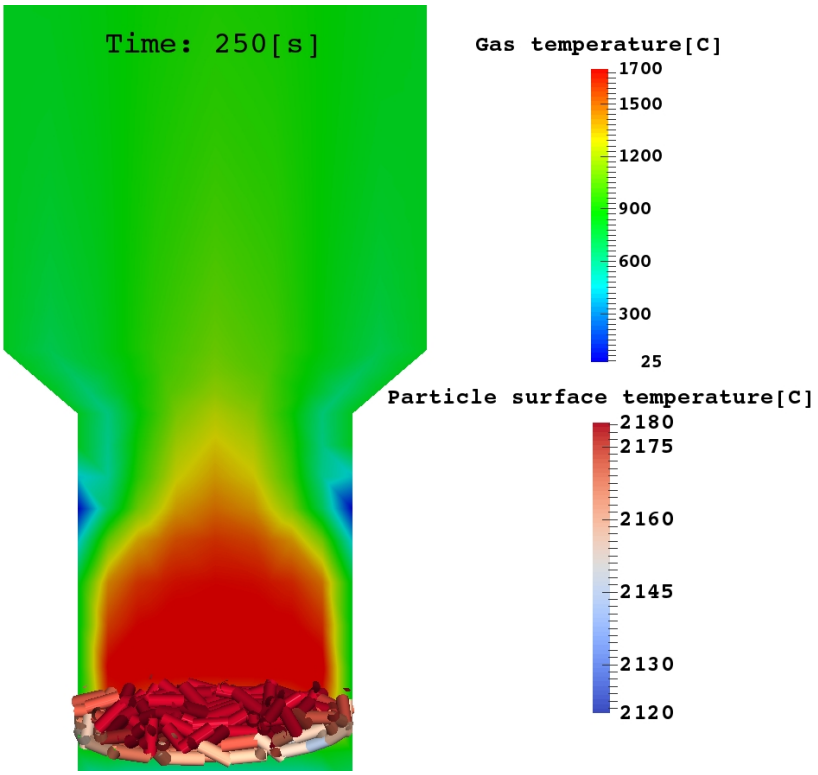

Figure 4: Temperature distribution of particles and gas flow at t=250s

4 CONCLUSIONS

The current contribution describes the Extended Discrete Element Method (XDEM) that is applied to thermal conversion of packed beds as often encountered in process engineering. The methodology relies on a Lagrange-Eulerian approach that couples effectively the particulate phase with a gas streaming through the void space of a packed bed reactor. The particle processes of the packed bed are described by the solution of one-dimensional and transient differential conservation equations for mass and energy. This set of equation is solved individually for each particle of the packed bed by fast and efficient algorithms. Thus, the thermodynamic state of each particle is determined taking into account space and time-dependent boundary conditions prevailing within the reactor such as heat and mass transfer between the particle surface and the surrounding gas phase. The latter is described by solving the conservation equations of classical Computational Fluid Dynamics (CFD). Hence, the numerical concept provide results over a large range of length scales ranging from inner particles processes to the global dimensions of the reactor. The presented approach deals with particle shapes of different sizes and takes heat and mass transfer between the particles surface and the surrounding gas phase into account that distinguishes the presented concept from current approaches. Thus, physics are described to a fine degree that allows an in-depth analysis of obtained results. It unveils the underlying physics of the processes involved and as a computer-aided tool contributes significantly to an improved design and operating conditions.

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